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Determination of Abraham Model Correlations for Solute Transfer into Propyl Acetate Based on Experimental Activity Coefficient and Solubility Data

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Abstract Experimental infinite dilution activity coefficients, gas-to-liquid partition coefficients, and molar solubility data have been measured for numerous organic solutes dissolved in propyl acetate. Results of our experimental measurements, combined with published solubility data retrieved from the published literature, have been used to derive Abraham model correlations for describing solute transfer into propyl acetate. The derived Abraham model correlations describe the experimental data to within 0.11 $\log_{10}$ units. Calculation of Abraham model solute descriptors for boscalid was illustrated using our derived solute transfer correlations into propyl acetate. Predictions using the calculated solute descriptors indicate that boscalid would show significant partitioning into the skin and fat tissues in the body, and would exhibit considerable baseline toxicity towards the eight aquatic organisms (five fish species and three water flea species).

Keywords Infinite dilution activity coefficients · Gas-to-organic solvent partition coefficients · Water-to-organic solvent partition coefficients · Molar solubilities · Aquatic toxicity · Blood-to-tissue partition coefficients

List of Symbols

a_k	Solvent property in Eq. 2 of the Abraham model reflecting the ability of the organic solvent to act as an H-bond acceptor
a_p	Solvent property in Eq. 1 of the Abraham model reflecting the ability of the organic solvent to act as an H-bond acceptor
b_k	Solvent property in Eq. 2 of the Abraham model reflecting the ability of the organic solvent to act as an H-bond donor

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